

4-(1-Cyanoethyl)-1,2,3,4-tetrahydronaphthalene-1-carbonitrile
57964-39-3 | DTXSID2057576

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 309 °C

Global applicability domain: Outside

Local applicability domain index: 3.37e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>(2-Chlorobenzylidene)propanedinitrile</div> <div>Measured: 313</div> <div>Predicted: 310</div>	<div>Image not found</div> <div>Chlorothalonil</div> <div>Measured: 350</div> <div>Predicted: 319</div>	<div>Image not found</div> <div>Acibenzolar-S-methyl</div> <div>Measured: 267</div> <div>Predicted: 295</div>
<div>Image not found</div> <div>1-Phenylimidazole</div> <div>Measured: 276</div> <div>Predicted: 273</div>	<div>Image not found</div> <div>1,5-Naphthalene diisocyanate</div> <div>Measured: 330</div> <div>Predicted: 319</div>	